

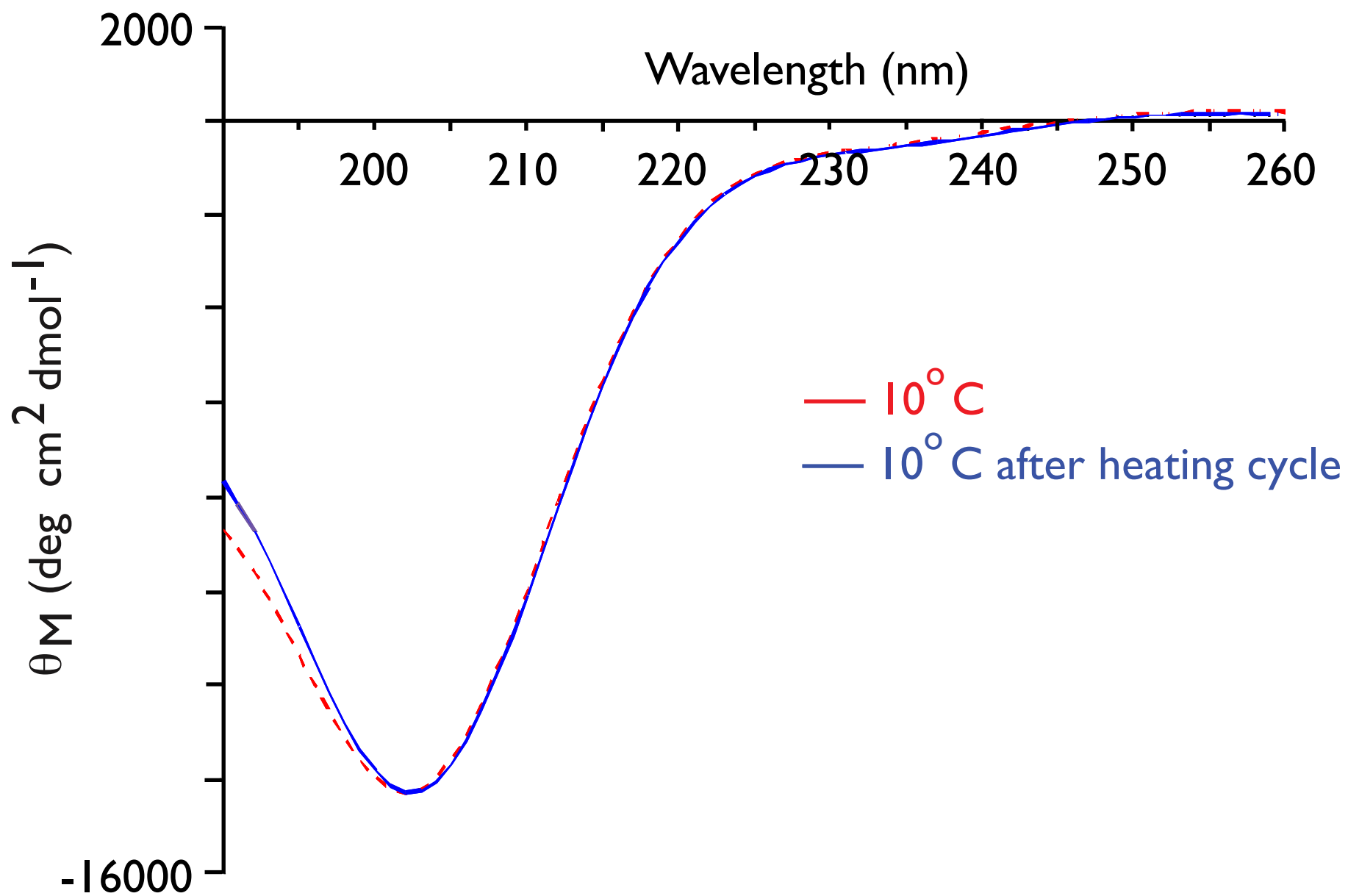
The tooth enamel protein, porcine amelogenin, is an intrinsically disordered protein with an extended molecular configuration in the monomeric form. Supporting Information.

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Supporting Figure S1: *Unquenched and quenched CD spectra of rPI 72 in UDDW.* Both spectra were recorded at 10° C with identical acquisition parameters. The red curve is the initial spectra of the sample (“unquenched”), the blue curve is the spectra obtained at 10° C after the initial sample was heated up up to 85° C, with subsequent cooling down to 10° C (“quenched”). The “quenched” spectrum is reproducible within the experimental error and indicates the absence of aggregation.



Residue	N _{alpha}	C _{alpha}	C=O	C _{beta}	C _{gamma}	C _{delta}	C _{epsilon}	C _{other}	NH	H _{alpha}	H _{beta}	H _{gamma}	H _{other}	³ J
P2	---	62.42	176.63	31.86	27.01	---	---	---	---	4.38	2.29	1.86	---	---
L3	124.20	52.87	177.07	41.41	---	---	---	---	8.42	3.97	---	---	---	7.8
P4	---	63.51	177.7	31.99	27.82	---	---	---	---	4.36	2.29	---	---	---
P5	---	63.51	177.7	31.99	27.82	---	---	---	---	4.36	2.29	---	---	---
H6	118.3	53.30	172.42	28.68	---	---	---	---	8.30	4.53	3.09	---	---	9.4
P7	---	63.44	177.47	32.08	27.52	---	---	---	---	4.23	2.17	1.86	---	---
G8	109.6	44.90	173.43	---	---	---	---	---	8.59	3.85	---	---	---	8.3
H9	118.3	53.3	172.42	28.84	---	---	---	---	8.30	4.53	3.09	---	---	9.4
P10	---	63.62	177.38	32.07	27.72	---	---	---	---	4.36	2.24	1.84	---	---
G11	109.83	45.05	173.65	---	---	---	---	---	8.65	3.85	---	---	---	7.2
Y12	120.02	57.85	175.51	38.84	---	---	---	---	8.03	4.50	2.87	---	---	---
I13	123.71	60.66	175.00	38.90	17.1	39.22	12.81	---	8.03	3.97	1.58	0.60	1.27, 0.60	10.1
N14	122.48	52.86	174.64	38.84	---	---	---	---	8.34	4.55	2.66	---	---	---
F15	121.54	58.00	175.43	39.69	---	---	---	---	8.21	4.45	2.89, 2.83	---	---	8.2
S16	117.21	58.05	173.86	63.71	---	---	---	---	8.14	4.32	3.87, 3.72	---	---	7.9
Y17	121.80	58.01	175.60	38.55	---	---	---	---	8.07	4.42	2.91	---	---	9.1
E18	122.02	56.30	175.96	30.28	---	---	---	---	8.23	4.49	2.14	1.86	---	---
V19	121.59	62.40	176.08	32.45	24.94	23.3	---	---	8.14	3.99	---	0.85	---	---
L20	125.80	55.06	177.07	42.29	---	---	---	---	8.35	4.39	1.60	1.48	0.78	7.2
T21	116.58	60.33	172.85	69.48	---	---	---	---	8.00	4.03	3.77	---	---	8.7
P22	---	63.62	177.38	27.57	---	---	---	---	---	4.35	2.26	1.85	---	---
L23	121.93	56.01	177.96	41.05	---	---	---	---	8.14	4.23	1.57	0.82	---	---
K24	120.67	57.14	177.13	32.81	---	---	---	---	8.12	4.21	3.14	1.65	---	---
W25	120.91	58.78	176.70	29.40	---	---	---	---	8.09	4.50	3.15	---	---	---

Residue	Nalpha	Calpha	C=O	Cbeta	Cgamma	Cdelta	Cepsilon	Cother	NH	Halpha	Hbeta	Hgamma	Hother	³ J
Y26	120.08	58.77	176.04	38.45	---	---	---	---	8.33	3.96	2.76	---	---	---
Q27	119.71	57.1	176.41	28.80	28.93	---	---	---	8.07	3.98	1.94	---	---	---
N28	117.75	54.04	175.51	38.46	---	---	---	---	8.18	4.50	2.72	---	---	7.8
M29	119.96	56.24	176.55	32.38	31.51	---	----	---	7.98	4.19	3.00	---	---	---
I30	120.24	61.62	176.23	38.05	27.10	13.01	---	---	8.03	3.97	1.58	0.60	---	---
R31	123.28	55.59	175.82	31.95	28.60	40.74	---	---	8.40	4.24	2.47	1.88	1.34	7.5
H32	119.47	52.98	172.03	28.57	---	---	---	---	8.38	4.53	3.09	---	---	---
P33	---	63.34	176.62	31.98	27.57	---	---	---	---	4.32	2.04	1.88	---	---
Y34	120.06	57.9	175.89	38.44	---	---	---	---	8.33	4.52	2.96	---	---	6.6
T35	115.66	61.4	174.00	70.09	21.27	---	---	---	7.93	4.03	3.77	---	---	9.2
S36	117.88	58.44	173.86	63.73	---	---	---	---	8.22	4.32	3.72	---	---	7.8
Y37	121.94	58.14	176.15	38.75	---	---	---	---	8.21	4.46	2.94, 2.84	---	---	---
G38	110.41	44.91	173.36	---	----	---	---	---	8.27	3.85	---	---	---	5.5
Y39	119.96	57.91	175.15	38.81	---	---	---	---	7.98	4.51	2.94	---	---	---
E40	N/O													---
c-P41	---	65.20	177.12	31.96	22.88	---	---	---	---	4.32	2.04	1.88	---	---
M42	120.32	56.07	177.08	31.96	---	---	---	---	8.53	4.25	2.47	1.96	---	---
G43	110.8	45.38	174.80	---	---	---	---	---	8.47	3.80	---	---	---	6.2
G44	108.71	45.10	174.07	---	---	---	---	---	8.20	4.01, 3.77	---	---	---	6.2
W45	120.06	57.71	176.72	29.4	----	---	---	---	8.09	4.50	3.15	---		6.2
L46	121.95	55.44	177.12	42.00	24.70	---	---	---	8.14	4.12	1.30	0.74	---	---
H47	117.83	55.06	174.11	28.63	---	---	---	---	8.29	4.53	3.09	---	---	9.3
H48	119.20	55.23	173.88	29.04	---	---	---	---	8.39	4.36	3.09	---	---	---

Residue	N α	C α	C=O	C β	C γ	C δ	C ϵ	C θ	NH	H α	H β	H γ	H θ	3J
I50	123.80	60.90	176.01	38.42	27.20	17.65	---	---	8.42	4.06	1.75	1.09	---	---
I51	128.18	60.90	174.29	38.42	27.20	17.65	---	---	8.39	4.06	1.75	1.09	---	9.4
c-P52	---	62.92	176.59	32.21	25.34	---	---	---	---	4.23	2.24	1.86	---	---
V53	121.59	62.30	176.59	32.72	20.89	---	---	---	8.32	4.02	1.97	0.85	---	---
V54*	121.30, 125.28	62.23	176.10	32.79	20.77	---	---	---	8.38	4.12	2.02	0.89	---	---
S55	120.42	58.29	174.57	63.77	---	---	---	---	8.51	4.39	3.80	---	---	6.8
Q56	122.76	55.83	175.84	29.45	33.66	30.63	---	---	8.56	4.30	2.31	1.86	---	8.2
Q57	121.86	55.64	175.95	29.48	33.79	29.49	---	---	8.52	4.33	2.31	2.01	---	---
T58	118.66	60.16	172.98	65.59	---	---	---	---	8.35	4.03	3.77	---	---	8.3
P59	---	63.47	177.08	32.08	27.57	---	---	---	---	4.35	2.26	1.85	---	---
Q60	120.74	55.94	176.20	29.38	29.17	---	---	---	8.58	4.23	2.34	1.96	---	---
S61	117.14	58.61	174.63	63.84	---	---	---	---	8.38	4.35	3.79	---	---	6.9
H62	120.66	55.09	174.01	29.00	---	---	---	---	8.58	4.66	3.23	---	---	---
A63*	124.71, 125.08	52.61	177.62	19.14	---	---	---	---	8.31	4.23	1.31	---	---	---
L64	121.81	54.95	177.29	42.18	27.09	24.69	23.55	---	8.35	4.33	1.56	0.86	---	7.3
Q65	122.51	53.64	173.87	28.89	29.20	---	---	---	8.44	4.23	2.25	1.88	---	---
P66	---	63.02	176.66	32.15	27.29	---	---	---	---	4.32	2.21	1.73	---	---
H67	118.55	55.19	174.28	29.02	---	---	---	---	8.68	4.57	3.11	---	---	7.6
H68	120.11	55.19	173.94	29.54	---	---	---	---	8.56	4.62	3.10	---	---	6.1
H69	121.48	55.35	173.98	29.25	---	---	---	---	8.78	4.61	3.10	---	---	8.0
I70	125.23	58.98	174.21	38.46	---	---	---	---	8.40	4.06	1.75	1.09	---	---
P71	---	63.04	176.55	32.17	27.29	---	---	---	---	4.32	2.21	1.73	---	---
M72	121.74	55.74	176.09	32.81	---	---	---	---	8.49	4.39	1.97	2.53	---	---
V73	124.00	59.79	174.31	32.71	---	---	---	---	8.32	4.12	2.02	0.89	---	7.8

Residue	N α	C α	C=O	C β	C γ	C δ	C ϵ	C θ	NH	H α	H β	H γ	H θ	3J
P74	---	63.14	176.51	32.14	27.34	---	---	---	---	4.35	2.26	1.90	---	---
A75	124.41	52.44	177.80	19.10	---	---	---	---	8.57	4.22	1.34	---	---	5.1
Q76	119.75	55.57	175.83	29.35	---	---	---	---	8.41	4.24	2.33	1.97	---	6.8
Q77	123.27	55.46	174.02	29.35	---	---	---	---	8.53	4.24	2.33	1.97	---	7.6
P78	---	63.32	177.35	32.13	27.71	---	---	---	---	4.39	2.26	1.91	---	---
G79	109.21	44.94	173.71	---	---	---	---	---	8.51	4.33, 3.88	---	---	---	5.8
I80	121.89	58.29	174.77	38.54	---	---	---	---	8.08	4.06	1.75	---	---	---
P81	---	63.23	176.77	32.07	27.47	---	---	---	---	4.33	2.26	1.93	---	---
Q82	121.11	55.67	175.92	33.91	29.49	---	---	---	8.57	4.26	2.30	1.86	1.63	7.0
Q83	123.36	53.92	173.88	28.97	---	---	---	---	8.54	4.26	2.30	1.86	1.63	7.2
P84	---	63.04	176.55	32.17	27.47	---	---	---	---	4.33	2.26	1.93	---	---
M85	121.74	55.74	176.09	32.81	---	---	---	---	8.49	4.39	1.97	2.53	---	---
M86	121.74	55.74	176.09	32.81	---	---	---	---	8.49	4.39	1.97	2.53	---	---
P87	---	62.42	176.63	31.86	27.01	---	---	---	---	4.39	2.26	1.93	---	---
L88	123.94	52.87	177.29	41.41	27.09	---	---	---	8.42	4.33	1.56	0.86	---	7.8
P89	---	63.51	177.70	31.99	27.82	---	---	---	---	4.36	2.29	1.93	---	---
G90	109.40	45.15	174.20	---	---	---	---	---	8.56	4.32, 3.88	---	---	---	7.9
Q91	119.51	55.72	175.97	33.67	29.01	---	---	---	8.17	4.25	2.27	1.97	---	8.0
H92	119.75	55.72	174.31	29.13	---	---	---	---	8.68	4.71	3.18	---	---	9.1
S93	117.27	58.43	174.45	63.74	---	---	---	---	8.46	4.41	3.81	---	---	7.3
M94	122.70	55.19	176.22	32.79	---	---	---	---	8.66	4.55	2.57	2.00	---	8.3
T95	118.71	60.12	172.87	69.59	---	---	---	---	8.35	4.31	4.10	1.12	---	8.5
c-P96	---	63.31	177.11	32.20	25.09	---	---	---	---	4.44	2.28	1.88	---	---
T97	115.18	62.18	174/49	69.70	---	---	---	---	8.33	4.31	4.10	1.12	---	8.4

Residue	N α	C α	C=O	C β	C γ	C δ	C ϵ	C θ	NH	H α	H β	H γ	H θ	3J
Q98	122.83	55.58	175.58	29.55	29.36	---	---	---	8.42	4.24	2.27	1.91	---	7.8
H99	120.04	55.58	174.07	29.13	---	---	---	---	8.64	4.60	3.11	---	---	8.8
H100	122.30	55.38	173.99	29.22	---	---	---	---	8.67	4.60	3.11	---	---	---
Q101	122.30	55.23	175.46	29.72	33.53	---	---	---	8.49	4.35	2.22	2.55, 1.88	---	---
P102	---	63.18	176.02	32.03	---	---	---	---	---	4.36	2.24	1.83	---	---
N103	118.76	53.15	174.72	38.82	---	---	---	---	8.58	4.61	2.72	---	---	---
L104	124.03	53.02	174.97	41.92	---	---	---	---	8.22	4.33	1.56	0.86	---	8.3
P105	---	62.42	176.63	31.86	27.01	---	---	---	---	4.38	2.24	1.83	---	---
L106	123.94	52.87	174.97	41.41	---	---	---	---	8.42	4.38	1.56	0.86	---	7.8
P107	---	63.14	176.51	32.14	27.34	---	---	---	---	4.35	2.26	1.90	---	---
A108	124.41	52.44	177.80	19.10	---	---	---	---	8.57	4.22	1.34	---	---	5.1
Q109	119.75	53.81	175.92	28.91	29.35	---	---	---	8.41	4.24	2.33	1.97	---	6.8
Q110	123.36	55.66	174.02	28.86	29.35	---	---	---	8.53	4.24	2.33	1.97	---	7.6
P111	---	63.27	176.39	32.15	27.21	---	---	---	---	4.42	2.51	2.03	---	---
F112	120.85	57.79	175.26	39.56	---	---	---	---	8.37	4.49	2.91	---	---	---
Q113	124.58	55.63	172.97	29.81	---	---	---	---	8.17	4.28	2.35	1.99	---	---
P114	---	63.12	176.80	32.05	27.21	---	---	---	---	4.36	2.28	1.87	---	---
Q115	120.94	55.63	175.91	32.28	---	---	---	---	8.60	4.28	2.35	1.99	---	---
P116	---	63.12	176.80	32.05	27.21	---	---	---	---	4.36	2.28	1.87	---	---
V117	124.00	62.29	176.20	31.70	20.89	---	---	---	8.32	4.00	1.97	0.90	---	---
Q118	126.03	53.52	173.88	28.97	---	---	---	---	8.59	4.28	2.35	1.99	---	7.7
P119	---	63.12	176.80	32.05	27.21	---	---	---	---	4.36	2.28	1.87	---	---
Q120	120.94	55.63	175.91	32.28	---	---	---	---	8.60	4.28	2.35	1.99	---	7.7
P121	--	63.12	176.08	32.05	27.21	---	---	---	---	4.36	2.28	1.87	---	---

Residue	N α	C α	C=O	C β	C γ	C δ	C ϵ	C θ	NH	H α	H β	H γ	H θ	3J
H122	120.69	55.38	173.99	29.22	---	---	---	---	8.67	4.60	3.11	---	---	---
Q123	122.30	55.23	175.46	29.72	---	---	---	---	8.49	4.35	2.22	2.55, 1.88	---	---
P124	---	63.12	176.80	32.05	27.21	---	---	---	---	4.36	2.28	1.87	---	---
L125	123.65	41.83	174.91		---	---	---	---	8.31	4.38	1.56	0.86	---	---
Q126	N/O													
P127	---	63.12	176.80	32.05	27.21	---	---	---	---	4.36	2.28	1.87	---	---
Q128	120.95	55.69	175.90	29.60	---	---	---	---	8.62	4.28	2.35	1.99	---	7.3
S129	117.17	63.21	176.63	32.82	---	---	---	---	8.50	4.26	3.77	---	---	---
c-P130	---	63.21	176.63	32.97	25.09	---	---	---	---	4.41	2.26	1.92	---	---
M131	120.93	56.07	175.96	32.81	29.79	19.5	---	---	8.54	4.30	2.29	1.94	---	---
H132	N/O													
t-P133	---	63.09	176.82	32.20	29.74	---	---	---	---	4.28	2.30	1.90	---	---
I134	121.99	61.20	176.25	38.68	27.27	17.65	13.75	---	8.47	4.09	1.78	1.17	---	---
Q135	126.11	53.38	173.71	28.97	---	---	---	---	8.52	4.28	2.35	1.99	---	---
P136	---	62.94	176.64	32.37	27.24	---	---	---	---	4.58	2.68	---	---	---
L137	120.67	55.14	177.10	42.34	27.00	24.57	---	---	8.47	4.27	1.56	0.87	---	---
L138	124.85	54.97	175.02	42.23	---	---	---	---	8.28	4.27	1.56	0.87	---	---
P139	---	63.12	176.80	32.05	27.21	---	---	---	---	4.36	2.28	1.87	---	---
Q140	120.94	55.63	175.91	32.28	---	---	---	---	8.52	4.28	2.35	1.99	---	---
P141	---	63.12	176.80	32.05	27.21	---	---	---	---	4.36	2.28	1.87	---	---
P142	---	62.42	176.63	31.86	27.01	---	---	---	---	4.38	2.28	1.87	---	---
L143	123.94	52.87	175.02	41.41	---	---	---	---	8.42	4.27	1.56	0.87	---	7.8
P144	---	63.14	176.51	32.14	27.34	---	---	---	--	4.35	2.26	1.90	---	---
P145	---	63.21	176.63	32.82	27.09	---	---	---	---	4.41	2.26	1.92	---	---

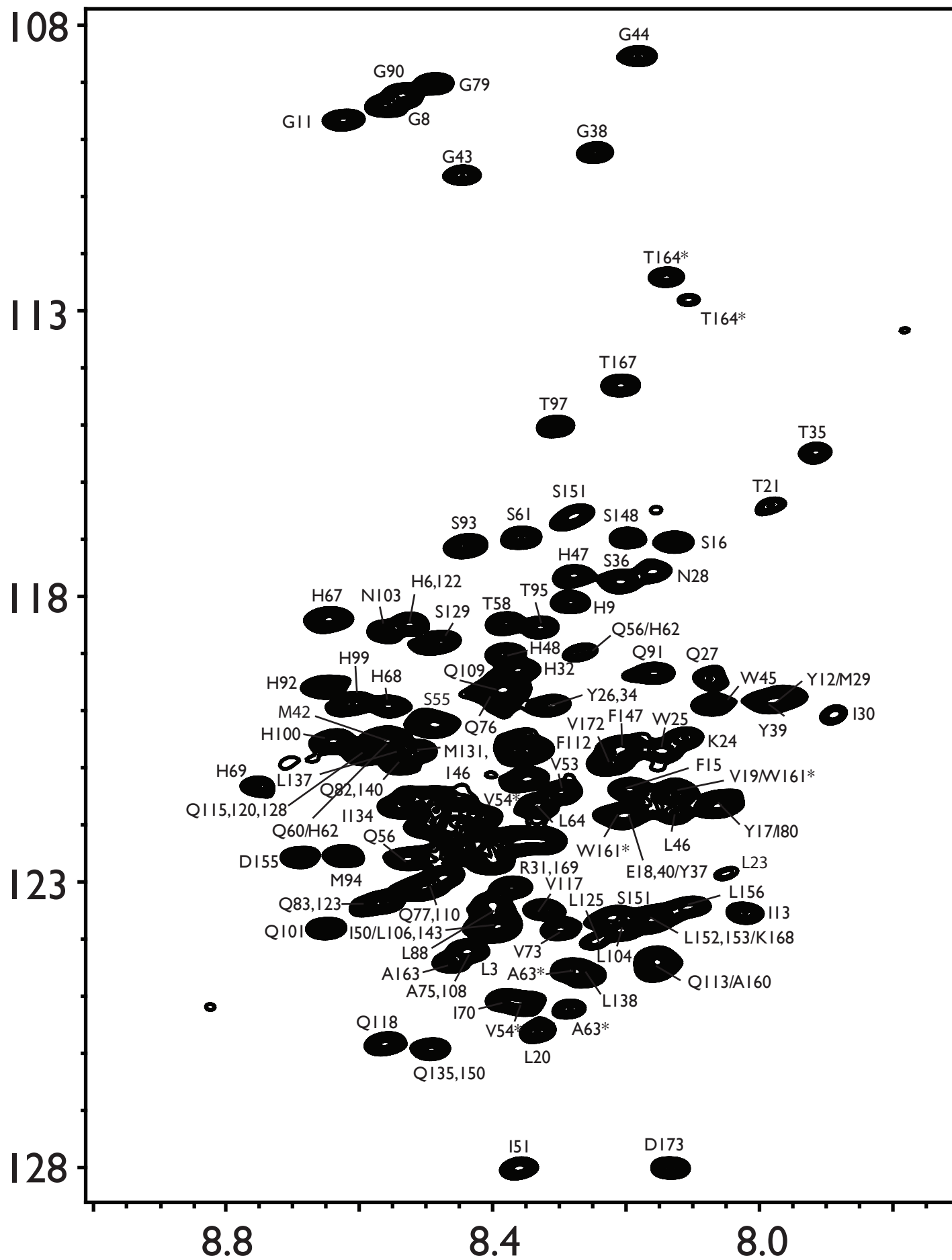
Residue	Nalpha	Calpha	C=O	Cbeta	Cgamma	Cdelta	Cepsilon	Cother	NH	Halpha	Hbeta	Hgamma	Hother	³ J
M146	120.93	56.07	175.96	32.81	29.79	19.50	---	---	8.54	4.30	2.29	1.94	---	---
F147	120.83	57.83	175.58	39.70	---	---	---	---	8.25	4.57	3.03	---	6.75	
S148	117.17	58.02	174.43	63.88	---	---	---	---	8.22	4.26	3.77	---	---	8.0
M149	122.41	56.07	175.96	32.81	---	---	---	---	8.44	4.30	2.29	---	---	---
Q150	126.04	59.30	176.66	59.30	33.64	---	---	---	8.52	4.25	2.3	2.0	---	8.0
S151	116.80	58.54	174.24	63.63	---	---	---	---	8.30	4.62	3.77	---	---	7.8
L152	123.85	55.12	177.04	42.24	25.06	23.30	21.53	26.83	8.18	4.27	1.56	0.87	---	---
L153	123.85	52.87	175.06	41.64	25.06	23.30	21.53	26.83	8.18	4.27	1.56	0.87	---	---
c-P154	---	62.1	172.42	32.43	26.38	---	---	---	---	4.35	2.40	1.99	---	---
D155	122.76	53.47	178.65	41.30	---	---	---	---	8.72	4.53	2.59	---	---	6.7
L156	123.63	53.00	175.04	41.77	---	---	---	---	8.12	4.27	1.56	0.87	---	8.0
P157	---	63.02	176.82	32.04	27.21	---	---	---	---	3.98	2.25	1.86	---	---
L158	122.41	55.17	177.55	42.30	---	---	---	---	8.34	4.42	1.59	0.85	---	---
E159	121.48	56.04	175.51	29.93	---	---	---	---	8.39	4.15	2.19	1.83		7.7
A160	124.60	52.56	176.90	19.39	---	---	---	---	8.17	4.21	1.21	---	---	---
W161*	121.50, 121.67	55.02	174.30	28.94	---	---	---	---	8.14, 8.20	4.50	3.15	---	---	---
P162	---	63.38	176.72	32.06	27.24				---	4.34	2.25	1.86	---	---
A163	124.60	52.64	178.21	19.13	---	---	---	---	8.47	4.32	1.39		---	---
T164*	112.57, 112.83	61.76	174.36	69.84	---	---	---	---	8.15, 8.09	4.33	4.15	1.19	---	8.6
D165	122.39	54.18	176.65	40.81	---	---	---	---	8.37	4.58	2.68		---	---
K166	122.58	56.63	177.10	32.57	29.01	24.81	---	---	8.47	4.28	1.90	1.75, 1.40	---	---
T167	114.47	62.67	174.68	69.59	---	---	---	---	8.23	4.17	1.21	---	---	8.0
K168	123.84	56.20	176.32	32.85	28.97	24.65	---	---	8.18	4.25	1.77	1.32	---	---

Residue	N α	C α	C=O	C β	C γ	C δ	C ϵ	C other	NH	H α	H β	H γ	H other	3J
R169	123.28	56.02	176.17	30.81	42.76	27.21	---	---	8.40	4.30	2.30	1.97	1.86, 1.61	7.5
E170	122.14	56.11	176.11	29.81	---	---	---	---	8.53	4.26	2.25	1.94	---	6.8
E171	122.06	56.23	175.92	29.83	---	---	---	---	8.45	4.30	2.26	1.92	---	---
V172	121.09	61.99	175.06	32.93	---	---	---	---	8.24	4.14	2.07	0.88	---	8.6
D173	128.18	---	179.89	---	---	---	---	---	8.14	---	---	---	---	---

Table S1: Temperature-corrected 15-N, 13-C, 1-H backbone, sidechain chemical shifts for 75 micromolar rP172 in UDDW, pH 3.8, 283 K (1-H 700 MHz)

All chemical shifts in ppm, 3J in Hz (obtained from HNHA experiments). Asterisk denotes residue with two crosspeaks on $^{15}\text{H}-^1\text{H}$ HSQC spectra identified in conformational exchange. N/O = not observed. Due to chemical shift overlap or other factors, sidechain ^{13}C and ^1H and 3J were not detected and thus could not be assigned; these are denoted by “---”. “Other” refers to higher order aliphatic, aromatic carbon or proton resonances beyond the gamma position. Where noted, certain Pro residues are categorized as the cis (“c”) or trans (“t”) configuration based upon database values for Pro $^{13}\text{C}\beta$, $^{13}\text{C}\gamma$ chemical shifts. Note that the M1 residue is absent in recombinant rP172.

Supporting Figure S2: Heteronuclear ^1H - ^{15}N HSQC spectrum of amelogenin rPI 72 in unbuffered deionized distilled water (UDDW). Spectra were obtained with 8 scans per increment, 1024 points in ω_2 (^1H), 256 increments in ω_1 (^{15}N), a recovery delay of 1 sec, a spectral window of 12 ppm in ω_2 and 24 ppm in ω_1 . Pulse widths were 8.62 μsec at -5 dB on the ^1H channel and 38 μsec at -2 dB on the ^{15}N channel. Decoupling was performed during acquisition using the GARP decoupling pulse train. Z-axis gradient parameters were of the sine.100 type. A sine-squared apodization function was used during processing. The size of the spectrum was 4096 by 1024 points, with zero-filling in both dimensions. The “*” symbol denotes duplicated HSQC resonances (V54,A63,W161,T164) that arise from conformational exchange.



Supporting Figure S3: *Expansion plot of the heteronuclear ^1H - ^{15}N HSQC spectrum of amelogenin rPI 72 in UDDW. Acquisition and processing parameters are identical to that described in Figure S2. The “*” symbol denotes duplicated HSQC resonances that are due to conformational exchange.*

